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APPLICATION NO.	FI	LING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/053,348		11/02/2001 Dan E. Rosenthal		020910-000310US	5933
26111	7590	05/03/2005		EXAMINER	
		R, GOLDSTEI 'ENUE, N.W.	PROCTOR, JASON SCOTT		
	GTON, DC 20005			ART UNIT	PAPER NUMBER
	,			2123	

DATE MAILED: 05/03/2005

Please find below and/or attached an Office communication concerning this application or proceeding.

	Application No.	Applicant(s)			
	10/053,348	ROSENTHAL, DAN E.			
Office Action Summary	Examiner	Art Unit			
	Jason Proctor	2123			
The MAILING DATE of this communication appears on the cover sheet with the correspondence address Period for Reply					
A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.  - Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.  - If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.  - If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.  - Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).  Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).					
Status					
1) Responsive to communication(s) filed on	_•	•			
2a) ☐ This action is <b>FINAL</b> . 2b) ☑ This	action is non-final.				
3) Since this application is in condition for allowa	Since this application is in condition for allowance except for formal matters, prosecution as to the merits is				
closed in accordance with the practice under Ex parte Quayle, 1935 C.D. 11, 453 O.G. 213.					
Disposition of Claims					
4)  Claim(s) 1-44 is/are pending in the application. 4a) Of the above claim(s) is/are withdrawn from consideration.  5)  Claim(s) is/are allowed.  6)  Claim(s) 1-44 is/are rejected.  7)  Claim(s) is/are objected to.  8)  Claim(s) are subject to restriction and/or election requirement.					
Application Papers					
9) ☐ The specification is objected to by the Examiner.  10) ☐ The drawing(s) filed on 19 June 2002 is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.  Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).  11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.					
Priority under 35 U.S.C. § 119					
<ul> <li>12) Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).</li> <li>a) All b) Some * c) None of:</li> <li>1. Certified copies of the priority documents have been received.</li> <li>2. Certified copies of the priority documents have been received in Application No.</li> <li>3. Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).</li> <li>* See the attached detailed Office action for a list of the certified copies not received.</li> </ul>					
Attachment(s)  1) Notice of References Cited (PTO-892) 2) Notice of Draftsperson's Patent Drawing Review (PTO-948) 3) Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08) Paper No(s)/Mail Date see attached.  4) Interview Summary (PTO-413) Paper No(s)/Mail Date.  5) Notice of Informal Patent Application (PTO-152) 6) Other:					

IDS dated 5/29/02, 7/30/02, 3/25/03, 2/23/04

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#### **DETAILED ACTION**

Claims 1-44 have been presented for examination. Claims 1-44 have been rejected.

#### **Priority**

Applicants' claim for priority under 35 U.S.C. § 119(e) to Provisional Applications No. 60/245,730; No. 60/245,688; No. 60/245,731; and No. 60/245,734, all filed on November 2, 2000 is acknowledged.

#### Specification

- 1. It has come to the Examiner's attention that Applicant has filed 41 pages of amendments to the original specification on June 19, 2002, but has also submitted a reformatted version of the original specification with proper margins on July 18, 2002 that does not represent the June 2002 amendments. The page and line numbers of the July 2002 specification do not correspond to the June 2002 amendments. Because these amendments are so numerous, the Examiner has not attempted to apply the June 2002 amendments to the July 2002 specification. The Examiner has applied the July 2002 amendments to the original specification for examination purposes only, however significant and numerous difficulties explained below still remain in the specification.
- 2. A substitute specification excluding the claims is required pursuant to 37 CFR 1.125(a) because numerous amendments to the specification do not clearly indicate the portions of the specification to be amended. The specification is therefore difficult to consider.

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A substitute specification must not contain new matter. The substitute specification must be submitted with markings showing all the changes relative to the immediate prior version of the specification of record. The text of any added subject matter must be shown by underlining the added text. The text of any deleted matter must be shown by strike-through except that double brackets placed before and after the deleted characters may be used to show deletion of five or fewer consecutive characters. The text of any deleted subject matter must be shown by being placed within double brackets if strike-through cannot be easily perceived. An accompanying clean version (without markings) and a statement that the substitute specification contains no new matter must also be supplied. Numbering the paragraphs of the specification of record is not considered a change that must be shown.

3. The use of several trademarks, such as Pentium® III (page 12), has been noted in this application. They should be capitalized wherever they appear and be accompanied by the generic terminology. Applicant is respectfully requested to review the disclosure in its entirety to identify and properly mark all trademarks.

Although the use of trademarks is permissible in patent applications, the proprietary nature of the marks should be respected and every effort made to prevent their use in any manner which might adversely affect their validity as trademarks.

4. The amendment filed June 19, 2002 is objected to under 35 U.S.C. 132(a) because it introduces new matter into the disclosure. 35 U.S.C. 132(a) states that no

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amendment shall introduce new matter into the disclosure of the invention. The added material which is not supported by the original disclosure is as follows: The amendment identified as beginning on page 5, line 24, changes an equation to an approximate equation. The amendment identified as beginning on page 11, line 23 amends material not present in the original specification. The amendment identified as beginning at page 13, line 31, materially changes the meaning of  ${}^{i}C^{k}(j)$ . The amendment identified as beginning at page 37, line 17 appears to amend more material than is indicated. See 37 CFR 1.121. This amendment materially changes the meaning of the three equations beginning on page 39, line 1. This amendment introduces a new equation. The amendment identified as beginning on page 42, line 13 materially changes the terms under discussion and creates difficulty regarding the first equation in that section. The amendment identified as beginning on page 44, line 7 materially changes the terms under discussion and creates difficulty regarding the first equation in that section.

- 5. Pages 11, 35, and 47 appear to be missing from the original specification but new material replacing those gaps appears to be present in the first substitute specification filed on July 18, 2002. Pages 11 and 47 have been amended. The amendment to page 47 appears to introduce new matter regarding the embodiments of the invention.
- 6. Numerous pages of the specification, including page 39, suffer from irregular line numbering, making it difficult to identify what is referred to by the amendment identified as beginning on page 39, line 13. Page 38 suffers from irregular line numbering,

making it difficult to identify what is referred to by the amendment identified as beginning on page 38, line 17.

7. Applicant is required to cancel the new matter in the reply to this Office Action.

# Claim Rejections - 35 USC § 101

#### 35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

8. Claims 1-44 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

#### MPEP 2111 reads as follows:

During patent examination, the pending claims must be "given \*>their< broadest reasonable interpretation consistent with the specification." > In re Hyatt, 211 F.3d 1367, 1372, 54 USPQ2d 1664, 1667 (Fed. Cir. 2000).< Applicant always has the opportunity to amend the claims during prosecution, and broad interpretation by the examiner reduces the possibility that the claim, once issued, will be interpreted more broadly than is justified. In re Prater, 415 F.2d 1393, 1404-05, 162 USPQ 541, 550- 51 (CCPA 1969) (Claim 9 was directed to a process of analyzing data generated by mass spectrographic analysis of a gas. The process comprised selecting the data to be analyzed by subjecting the data to a mathematical manipulation. The examiner made rejections under 35 U.S.C. 101 and 102. In the 35 U.S.C. 102 rejection, the examiner explained that the claim was anticipated by a mental process augmented by pencil and paper markings. The court agreed that the claim was not limited to using a machine to carry out the process since the claim did not explicitly set forth the machine. The court explained that "reading a claim in light of the specification, to thereby interpret limitations explicitly recited in the claim, is a quite different thing from reading limitations of the specification into a claim,' to thereby narrow the scope of the claim by implicitly adding disclosed limitations which have no express basis in the claim." The court found that applicant was advocating the latter, i.e., the impermissible importation of subject matter from the specification into the claim.). See also In re Morris, 127 F.3d 1048, 1054-55, 44 USPQ2d 1023, 1027-28 (Fed. Cir. 1997)

## MPEP 2106 (IV)(B)(1) reads as follows:

If the "acts" of a claimed process manipulate only numbers, abstract concepts or ideas, or signals representing any of the foregoing, the acts are not being applied to appropriate subject matter. Schrader, 22 F.3d at 294-95, 30 USPQ2d at 1458-59. Thus, a process consisting solely of mathematical operations, i.e., converting one set of numbers into another set of numbers, does not manipulate appropriate subject matter and thus cannot constitute a statutory process.

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9. Claims 1-8, 17-22, 29-30, 33-34, and 37-40 are directed to a method which is merely a mathematical algorithm and therefore nonstatutory. These claims do not recite any machinery to carry out the process and are therefore not directed to the technological arts. Such a process does not manipulate appropriate subject matter and thus cannot constitute a statutory process. The Examiner respectfully suggests claiming these methods as computer-implemented methods as well as including a concluding step in independent claims 1, 5, 17, and 21 that distinguishes these methods from purely abstract mathematical methods. Generating a matrix or a partition of a matrix is considered a step of a mathematical algorithm.

### MPEP 2106 (IV)(B)(1) reads as follows:

Claims to computer-related inventions that are clearly nonstatutory fall into the same general categories as nonstatutory claims in other arts, namely natural phenomena such as magnetism, and abstract ideas or laws of nature which constitute "descriptive material." Abstract ideas, Warmerdam, 33 F.3d at 1360, 31 USPQ2d at 1759, or the mere manipulation of abstract ideas, Schrader, 22 F.3d at 292-93, 30 USPQ2d at 1457-58, are not patentable. Descriptive material can be characterized as either "functional descriptive material" or "nonfunctional descriptive material." In this context, "functional descriptive material" consists of data structures and computer programs which impart functionality when employed as a computer component. (The definition of "data structure" is "a physical or logical relationship among data elements, designed to support specific data manipulation functions." The New IEEE Standard Dictionary of Electrical and Electronics Terms 308 (5th ed. 1993).) "Nonfunctional descriptive material" includes but is not limited to music, literary works and a compilation or mere arrangement of data. Both types of "descriptive material" are nonstatutory when claimed as descriptive material per se. Warmerdam, 33 F.3d at 1360, 31 USPQ2d at 1759.

10. Claims 9-16, 23-28, 31-32, 35-36, and 41-44 are directed to *computer code* and are therefore nonstatutory. Functional descriptive material is nonstatutory when claimed as descriptive material. The Examiner respectfully suggests directing these claims to computer code tangibly embodied as part of a computer system that configures the system to perform the recited methods.

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11. To expedite a complete examination of the instant application the claims rejected under 35 U.S.C. § 101 (nonstatutory) above are further rejected as set forth below in anticipation of applicant amending these claims to place them within the four statutory categories of invention.

# Claim Rejections - 35 USC § 112

The following is a quotation of the first paragraph of 35 U.S.C. § 112:

The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

- 12. Claims 33-36 are rejected under 35 U.S.C. § 112, first paragraph, as failing to comply with the enablement requirement. The claim(s) contains subject matter which was not described in the specification in such a way as to enable one skilled in the art to which it pertains, or with which it is most nearly connected, to make and/or use the invention.
- 13. These claims recite limitations related to the precision of numerical and analytical Jacobian matrices. Claims 33 and 34, depending from the abstract mathematical methods of claims 1 and 5 respectively, refer to the precision of an abstract analytical computation. Such a computation is well known in the art to be completely precise. For example, the computation  $2 \cdot \pi = 2\pi$  to an infinite number of digits. There is no error in an analytic calculation; it has perfect precision. In contrast, the numeric computation  $2 \cdot \pi = 2 \cdot 3.14 = 6.28$  is accurate to two digits. By relating the number of accurate digits

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in the numeric computation to the analytic computation, these claims encompass

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completely precise numeric computation. A person of ordinary skill in the art would be

unable to make and use an invention that makes use of completely precise numeric

computation.

14. Claims 35 and 36, depending from the computer code of claims 9 and 13

respectively, refer to the precision of the implementation dictated either by the code

itself or by the machine on which the code is executed. Applicants' disclosure describes

an abstract mathematical algorithm but does not teach an implemented algorithm for

that method which accounts for the sources of numerical instability (which directly

determine the number of accurate digits) when executed on a computational machine.

Development of numerically stable implementations of complex algorithms is a science

to itself and requires great levels of experimentation and testing to achieve results. A

person of ordinary skill in the art would not be able to make and use an invention that

requires numerical stability for a complex abstract algorithm where no implementation is

taught without undue experimentation.

15. If claims 1 and 5 were amended to be statutory as computer-implemented

methods, claims 33 and 34 would be rejected for the reasons given regarding claims 35

and 36 above.

The following is a quotation of the second paragraph of 35 U.S.C. § 112:

The specification shall conclude with one or more claims particularly pointing out and distinctly claiming the subject matter which the applicant regards as his invention.

- 16. Claims 17-28 are rejected under 35 U.S.C. § 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.
- 17. Independent claims 17, 21, 23, and 27 recite mathematical expressions which have numerous unspecified elements. The elements of the Jacobian matrix *J* are described in written language however the equations of motion, necessary to achieving successful use of the claimed invention according to Applicants' method, are not provided until dependent claims 18, 22, 24, and 28. In contrast, claims 3, 7, 11, and 15 provide adequate description of the Jacobian matrix as well as the necessary equations of motion in the same claim. Mathematical expressions that contain expressions or variables that are inadequately defined are vague and indefinite and do not establish the metes and bounds of patent protection sought.
- 18. Claims 19-20 and 25-26 are rejected under 35 U.S.C. § 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.
- 19. Claims 19 and 25 recite the limitation "reducing said number of atoms to a smaller number of rigid bodies so as to reduce the number of computations for Jacobian partitions  $J_{uq}$  and  $J_{uu}$ ". The meaning of this phrase is unknown. Presumably "reducing said number of atoms" would result in fewer atoms, not a smaller number of rigid bodies. It appears that this limitation removes atoms from the rigid body model,

however this interpretation seems unlikely in light of the nature of the invention.

Clarification is required.

- 20. The term "approximately" in claims 20 and 26 is a relative term which renders the claim indefinite. The term "approximately" is not defined by the claim, the specification does not provide a standard for ascertaining the requisite degree, and one of ordinary skill in the art would not be reasonably apprised of the scope of the invention.
- 21. Further, it is unknown what is meant by the phrase "said number of computations is reduced approximately by the average number of atoms in each of said rigid bodies". It is unclear how the number of atoms in the rigid bodies is related to the number of computations. The number of computations is clearly related to the number of rigid bodies.
- 22. Claims 21-22 are rejected under 35 U.S.C. § 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.
- 23. Claim 21 appears to have a typographical error in line 3: "selecting a torsion angle, rigid multibody model for said physical; and". The Examiner presumes this should read "said physical system", however line 4 makes reference to "said physical model". There is clear antecedent basis for "rigid multibody model", but there is not antecedent basis for "physical model". Presumably "physical model" is a reference to "rigid multibody model of the physical system", however this would be speculation. Appropriate correction is required.

- 24. Claims 29-32 are rejected under 35 U.S.C. § 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.
- 25. These claims recite a relationship between the number of computations required to compute the analytical Jacobian matrix and the number of computations required to compute the numerical Jacobian matrix. This relationship is defined by the number N, where "N is proportional to the number of rigid bodies in said model". The indefiniteness regarding the value of N renders the claim indefinite because it is impossible to determine how many computations are involved for either the analytical or numerical Jacobian matrix. The Examiner is intimately familiar with algorithm analysis and Big-Oh notation, however, here there is no definite relationship between the number of rigid bodies in the model and the number of computations. Defining the relationship as "proportional" is far too broad to allow an adequate analysis of the prior art.
- 26. Further, the exponent p is not defined in these claims. Mathematical expressions that contain expressions or variables that are inadequately defined are vague and indefinite and do not establish the metes and bounds of patent protection sought. The relationship presented in these claims between the number of computations required for the analytical and numerical Jacobians is so broad that it would cover any relationship in the prior art and therefore claims a mathematical fact.

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- 27. Claims 33-36 are rejected under 35 U.S.C. § 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.
- 28. These claims recite limitations related to the precision of numerical and analytical Jacobian matrices. In particular, that the calculation of a numerical Jacobian has an accuracy of K digits while calculation of the analytical Jacobian has 2K digits. If claims 1, 5, 9, and 13 were amended to be statutory, these claims would refer to the precision and accuracy of either the implementation of the algorithm or the machine on which the code is executed. The disclosure does not teach any specific implementation or machine, however the Pentium® III or Pentium® 4 are exemplary machines (page 12, lines 18-22). It is impossible to determine the metes and bounds of these limitations if the implementation is, for example, a 64-bit architecture such as a SPARC® processor. Adding to the indefiniteness of these limitations are Fig. 7 and related (page 46, lines 1-5) which appear to teach that the numerical computation achieves as many as 8 digits of accuracy while the analytic computation achieves 15. It is unclear whether these claims exclude those perturbations where the numerical computation achieves 8 digits of accuracy or if the disclosure intends to have some other teaching.
- 29. Further, it is impossible to determine the metes and bounds of these claims because it is unclear if the accuracy of the computation is intended to be a feature of the claimed method, a feature of an implementation of the method, or a feature of the machine on which the code is executed.

## Claim Interpretation

In the interest of compact prosecution, the Examiner makes the following claim interpretations in order to apply prior art to the claims. See *Ex parte lonescu*, 222 USPQ 537 (Bd. Pat. App. & Inter. 1984).

- 30. In general, the state of the claims in the instant application precludes a limitation-by-limitation assessment of the claimed invention compared to the prior art. The Examiner cannot interpret the meanings of several claims without relying on speculation. See *In re Steele*, 305 F.2d 859,134 USPQ 292 (CCPA 1962).
- 31. Claims 1-4, 29, 33, 37, and 38 are considered exemplary of the other claims presented. The meaning of claims 29 and 33, which depend from claim 1, cannot be interpreted without significant speculation. Clarification of these claims would be greatly appreciated. The Examiner cannot perform a meaningful analysis of claims 29 and 33 (similarly claims 30-32 and 34-36) regarding novelty or non-obviousness and therefore they have not been treated on the merits.
- 32. As a result, the claims have been interpreted along the lines of 1-4, 37, and 38, although in anticipation that they will be amended to place them within the four categories of statutory invention, and with their respective embodiments as computer-implemented methods, computer systems, et cetera.

### Claim Objections

33. Applicant is advised that should claims 1-4, 29, 33, and 37-38 be found allowable, claims 9-12, 31, 35, and 41-42 will be objected to under 37 CFR 1.75 as

being a substantial duplicate thereof. When two claims in an application are duplicates or else are so close in content that they both cover the same thing, despite a slight difference in wording, it is proper after allowing one claim to object to the other as being a substantial duplicate of the allowed claim. See MPEP § 706.03(k). The first group of claims recite a method that the Examiner anticipates will be made statutory by being amended to be a computer-implemented method. The second group of claims recites computer code that the Examiner anticipates will be made statutory be being tangibly embodied in a computer system, thus the invention will be defined by the computer-implemented method it performs.

- 34. Claims 5-8, 30, 34, and 39-40 are similarly substantial duplicates of claims 13-16, 32, 36, and 43-44.
- 35. Similar objections may be required for claims 17-20, 21-22, 23-26, and 27-28 as substantial duplicates of claims 1-4 and/or 5-8 once the numerous rejections under 35 U.S.C. § 112, first and second paragraphs, have been resolved.

# Claim Rejections - 35 USC § 103

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

- (a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negatived by the manner in which the invention was made.
- 36. Claims 1-2, 5-6, 9-10, 13-14, 17, 21, 23, 27, 37, 39, and 41 are rejected under 35 U.S.C. § 103(a) as being unpatentable over "SD/FAST User's Manual Version B.2"; by

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Hollars et al.; September 1996; hereafter referred to as SD/FAST (supplied by Applicant in Information Disclosure Statement submitted on March 31, 2003) in view of "Integration methods for molecular dynamics"; by Benedict J. Leimkuhler, Sebastian Reich, and Robert D. Skeel; November 16, 1994; hereafter referred to as Skeel.

Regarding claims 1, 9, 17, and 23 SD/FAST teaches a computer system that performs rigid body analysis and modeling of a physical system (pages T-1, T-2). SD/FAST teaches modeling large systems (300 rigid bodies) and flexible bodies represented by a set of rigid bodies connected by joints (page T-11), which would be obviously similar to a molecule to a person of ordinary skill in the art. SD/FAST teaches applying forces and torques to the model (pages T-12, T-13), which would be obviously applicable to a torsion angle to a person of ordinary skill in the art. SD/FAST teaches performing a kinematic and dynamic motion analysis with several methods including numerical analysis (pages T-14, T-15, T-16). SD/FAST teaches routines for producing equations of motion, including Jacobian Systems (pages R-24, R-25, R-26).

SD/FAST does not explicitly teach implicit integration among the several methods of analysis.

Skeel teaches various integration methods for molecular dynamics including implicit methods (page 9). Skeel teaches that implicit methods have several advantages including being symplectic, time-reversible, and second order accurate. Skeel teaches that implicit methods enable much larger time steps. It would have been obvious to a person of ordinary skill in the art to combine an implicit method of integration as taught by Skeel with the rigid body analysis and modeling system

SD/FAST in order to create an analysis that is symplectic, time-reversible, second order accurate, and enjoys much larger time steps. This combination could be achieved by implementing an implicit integration method among the analysis methods already incorporated into SD/FAST. It would have been obvious to a person of ordinary skill in the art at the time of Applicants' invention to model molecular dynamics as a physical system in SD/FAST as a result of his own knowledge of the particular art as well as the nature of the problem to be solved.

37. Regarding claims 2, 6, 10, 14, 37, 39, 41, and 43, it would have been obvious to a person of ordinary skill in the art to form the equations of motion from either the Direct Form or the Residual Form of the equations of motion depending on the nature of the problem to be solved. Skeel teaches decoupling the equations of motion into a set of independent harmonic oscillators, allowing one to focus on whichever modes are of interest (pages 9-10). It would have been obvious to a person of ordinary skill in the art at the time of Applicants' invention to focus on the portions of the equations of motion that relate to the nature of the problem to be solved.

# Allowable Subject Matter

38. Claims 3-4, 7-8, 11-12, 15-16, 18-20, 22, 24-26, and 28 are objected to as being dependent upon a rejected base claim, but would be allowable if rewritten in independent form including all of the limitations of the base claim and any intervening claims. The determination of allowable subject matter is based on the Examiner's

interpretation of these claims in light of the numerous rejections under 35 U.S.C. §§ 101 and 112 above. Claims 19-20 and 25-26 will be given particular scrutiny regarding their difficulties under 35 U.S.C. § 112.

39. The following is a statement of reasons for the indication of allowable subject matter: Although the concept of rigid body modeling of a molecule, broadly referred to in the art as rigid body molecular dynamics, is well known, a search of the prior art has failed to uncover the claimed equations of motion or their equivalent as recited by exemplary claim 3. The prior art does not render obvious the steps necessary to modify the known equations of motion to arrive at the particular equations recited by exemplary claim 3.

## Conclusion

Art considered pertinent by the examiner but not applied has been cited on form PTO-892.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Jason Proctor whose telephone number is (571) 272-3713. The examiner can normally be reached on 8:30 am-4:30 pm M-F.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Kevin J Teska can be reached on (571) 272-3716. The fax phone number for the organization where this application or proceeding is assigned is (571) 273-3713.

Any inquiry of a general nature or relating to the status of this application should be directed to the TC 2100 Group receptionist: 571-272-2100. Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see http://pair-direct.uspto.gov. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

Jason Proctor Examiner Art Unit 2123

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